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Consistent vapour-liquid equilibrium data containing lipids

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Consistent physical and thermodynamic properties of pure components and their mixtures are important for process design, simulation, and optimization as well as design of chemical based products. In the case of lipids, it was observed a lack of experimental data for pure compounds and also for their mixtures in open literature, what makes necessary the development of reliable predictive models based on limited data. To contribute to the missing data, measurements of isobaric vapour-liquid equilibrium (VLE) data of three binary mixtures at two different pressures were performed at State University of Campinas (UNICAMP – Brazil), using Differential Scanning Calorimetry (DSC) technique, i.e., monoacylglycerol + fatty acid (system 1), monoacylglycerol + fatty ester (system 2) and monoacylglycerol + glycerol (system 3). System 1 is relevant in the purification steps of the deodorizer distillates while systems 2 and 3 are relevant in the purification steps of biodiesel and bioglycerin. It should be highlighted that there is no such data in the open literature, not only for the specific compounds we selected but also for the combination of the classes of compounds considered in this work.

Available thermodynamic consistency tests for TPx data were applied before performing parameter regressions for well-known thermodynamic models such as Wilson, NRTL, UNIQUAC and UNIFAC. In the pure compound consistency test ($Q_{\text{test},5}$ of TDE program developed at NIST), the consistencies of the end-points ($x=0$ and 1) of the VLE data are considered by comparing these values with their pure compound vapor pressures. Van Ness test where also considered in this work ($Q_{\text{test},1}$ of program TDE developed at NIST), that check how the measured data represent the thermodynamic models. Boiling temperatures and vapor phase compositions were calculated using Wilson, NRTL, UNIQUAC, and original UNIFAC models and bubble-point calculations. The relevance of enlarging experimental databank of lipids systems data in order to improve the performance of predictive thermodynamic models was confirmed in this work by analyzing the calculated values of original UNIFAC model and by proposing new interaction parameters for UNIFAC model and lipids systems. Also PC-SAFT model were analysed for lipids and a modification is proposed.